Preparing Exercise I-3: Optimization of cross-section tables using sensitivity coefficients in COBAYA3

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Introduction

- One of the objectives of Exercise I-3 (Core Physics) – UAM consists of performing core calculations to propagate the homogenized XS uncertainties to core parameters (k-eff, ...)
- Nodal diffusion codes are the most common option for 3D LWR core neutronics analysis
- Recently, within COBAYA3 it has been implemented the adjoint flux calculation capability for the steady state diffusion equation ⇒ sensitivities of k-eff to XS can be obtained

$$\frac{\partial k}{\partial \Sigma_a^g} = \frac{k^2}{\left\langle \vec{\phi}^* \middle| \vec{\chi} \cdot \sum_{\forall g'} \upsilon \Sigma_f^{g'} \cdot \phi^{g'} \right\rangle} \iiint_P \phi^{*g} \phi^g d\vec{r} \qquad \frac{\partial k}{\partial \upsilon \Sigma_f^g} = \frac{k}{\left\langle \vec{\phi}^* \middle| \vec{\chi} \cdot \sum_{\forall g'} \upsilon \Sigma_f^{g'} \cdot \phi^{g'} \right\rangle} \sum_{\forall g'} \iiint_P \phi^{*g'} \cdot \chi^{g'} \cdot \phi^g d\vec{r}$$

- They could be employed for:
  - ✓ Uncertainty propagation (UAM)
  - ✓ Optimization studies ⇒ used in the XS libraries building

Introduction

- Few-group homogenized cross section libraries are the input data of nodal diffusion codes

- Those data are generated by a lattice code for certain combination of state-variables, i.e. temperatures or densities and its accuracy strongly influences the accuracy of the reactor core calculation

- Depending on the way of compile the XS two types of data libraries can be found: multidimensional tables and parameterized libraries (functional fitting)

Introduction

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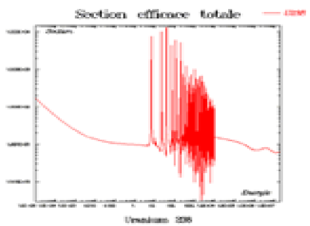
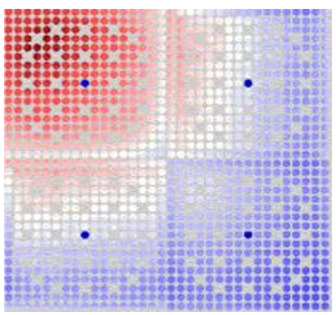


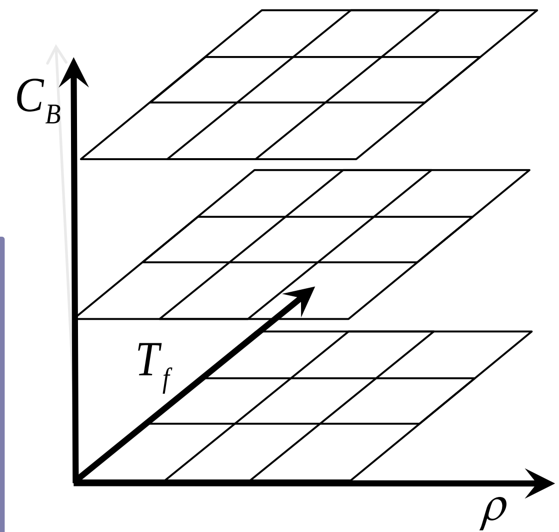
Lattice code



Condensation and homogenization

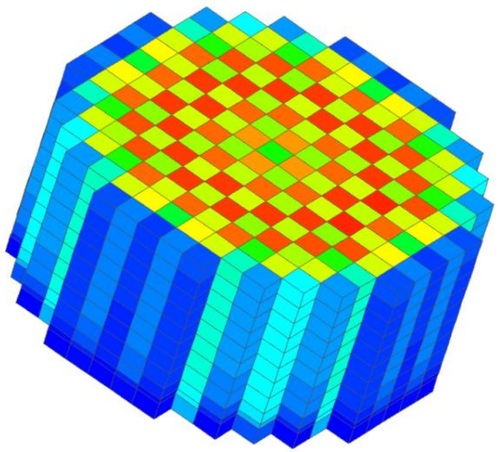
LIBRARIES

$$\Sigma\left(Q, T_m, T_f, \rho, C_B, ..\right)$$



Σ

Nodal diffusion 3D calculation



$$\Sigma(Q, T_f, T_m, C_B, \rho_m) = a_0 + a_1\rho + a_2\rho^2 + .. + b_1 C_B + .. + c_1 \rho \cdot C_B + ..$$

Objective

- Multi-dimensional tabulated libraries are the most straightforward form of cross section compilation (Advantage: no functional-fitting procedure)
- During the core calculation an interpolation algorithm is used to compute the cross sections at any state from the values at the mesh points
- The interpolation process introduces an error $\Rightarrow$ necessity of refining the mesh to assure a level of accuracy (Drawbacks: $\uparrow$ storage size and $\uparrow$ lattice calculations)
- However, k-eff constant is not equally sensitive to changes of different XS over the entire domain of the state variables $\Rightarrow$ the mesh should be refined only when necessary
- Main objective: Development of a methodology to optimize nodal XS tabulated libraries with the minimum number of mesh points for each state variable satisfying a user-given accuracy in k-effective constant

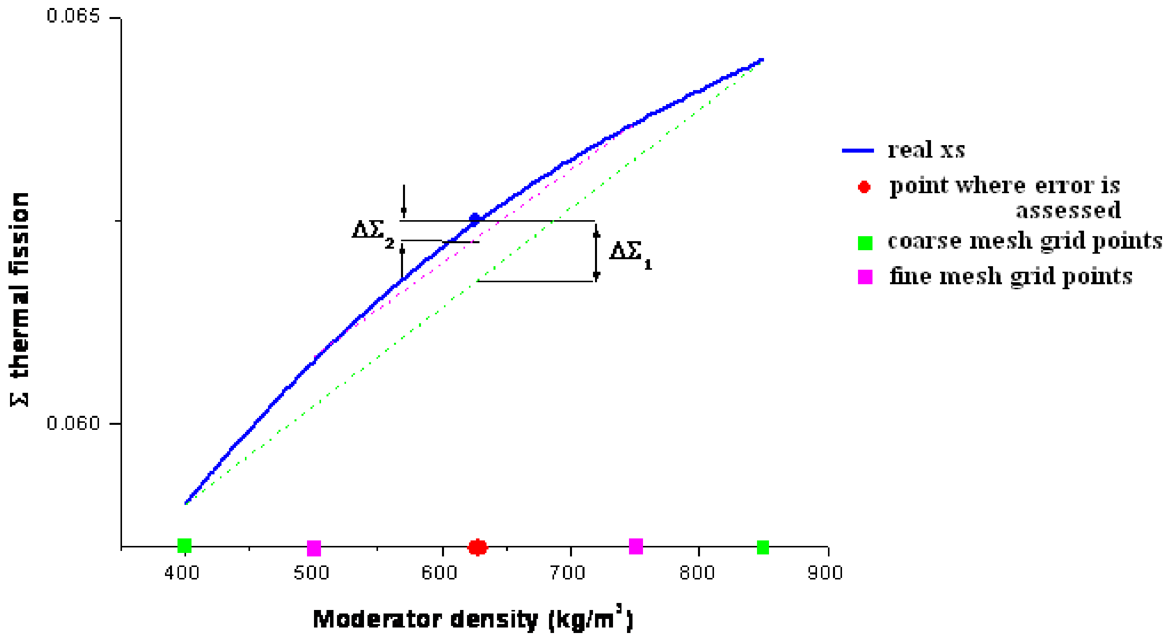
Objective

Statement of the problem

- The interpolation error on a given value of the state variable, i.e. moderator density, is defined as:

$$\varepsilon(\rho) = \left|\Sigma(\rho) - P(\rho)\right| \qquad P(\rho) = \sum_{i=1}^{N+1} a_i \rho^{i-1}$$

- The error depends on the type of interpolation (cubic, spline, …) and also on the grid coordinates (points between the interpolation is done)



Objective

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- The objective is not find the set of data-points that minimize the error over the variable domain; but the data-points that lead to XS errors with a limited impact on the parameters of interest, such as k-eff

Optimization process

- First, a user-given level of accuracy in k-eff terms is specified:

$$\left|\Delta k\right| \leq 10\,pcm$$

- Sensitivity coefficient of k-eff with respect to each cross section is computed (first order perturbation theory):

$$S_{\Sigma}^{k} = \frac{\delta k}{\delta \Sigma}$$

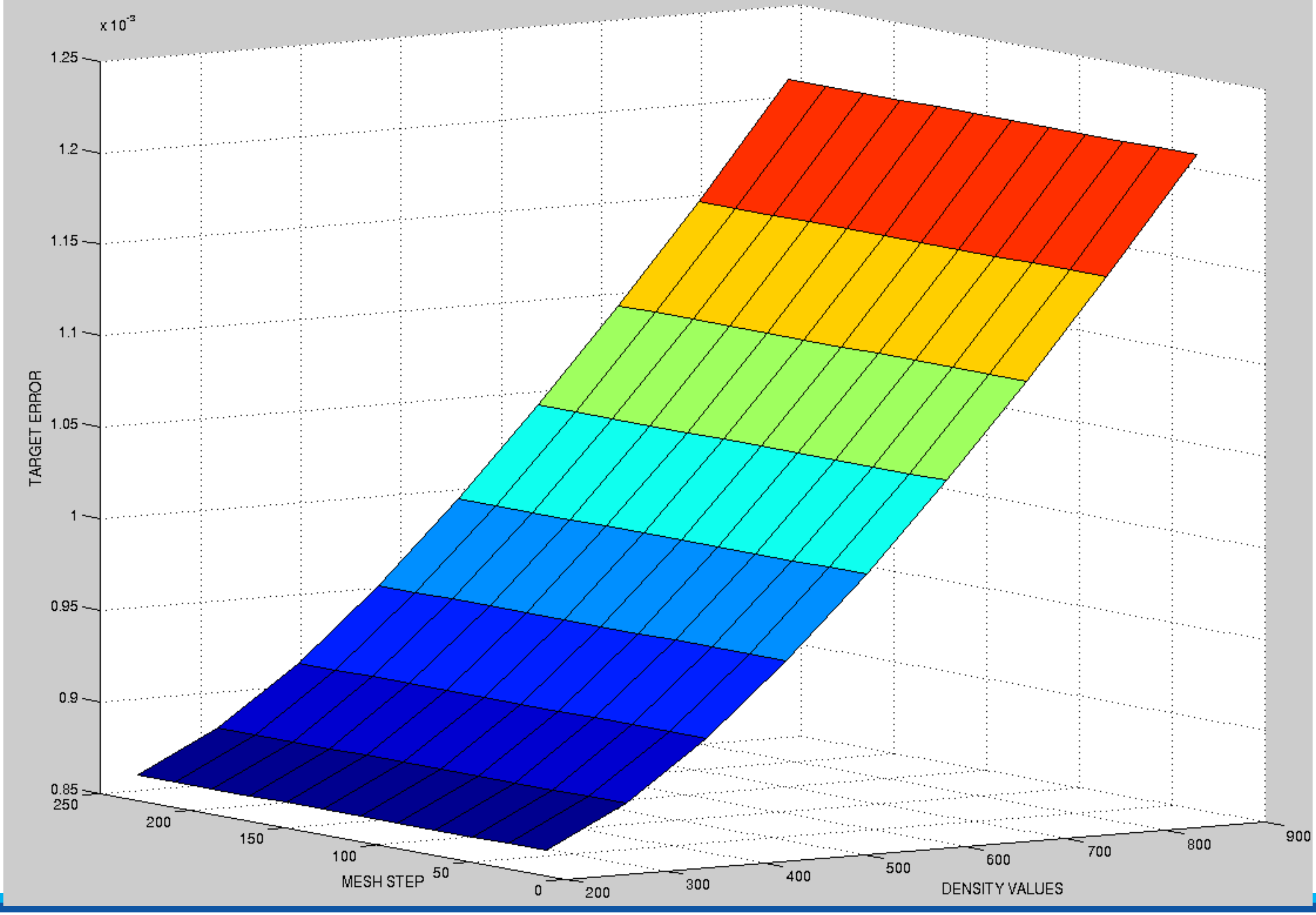
- The maximum allowed error in the XS can be assessed. If we assume only dependency on one XS:

$$\left|\Delta k\right| = S_{\Sigma}^{k}\left|\Delta\Sigma\right| \qquad \varepsilon_{\text{target}} = \left|\Delta\Sigma\right| = \frac{\left|\Delta k\right|}{\left|S_{\Sigma}^{k}\right|} \leq \frac{10^{-4}}{\left|S_{\Sigma}^{k}\right|}$$

- That is, a target error function for each cross section is defined, which depends on the state variable

$$\varepsilon_{\text{target}} = f(\rho)$$

Optimization process



Optimization process

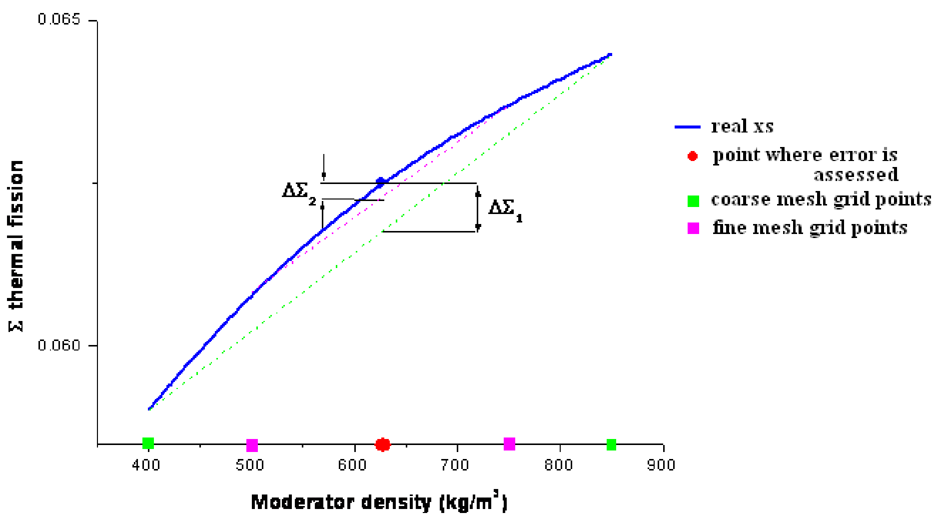
- The error due to the interpolation algorithm is calculated at different state values (different from grid coordinates) using different mesh steps
- This error can be expressed as a function of two variables:

$$\varepsilon_{\text{int}} = f(\rho, \Delta\rho)$$

$$\varepsilon_{\text{int}1}(\rho_1) = \Sigma(\rho_1) - \sum_{i=1}^{N+1} a_i \rho^{i-1}$$

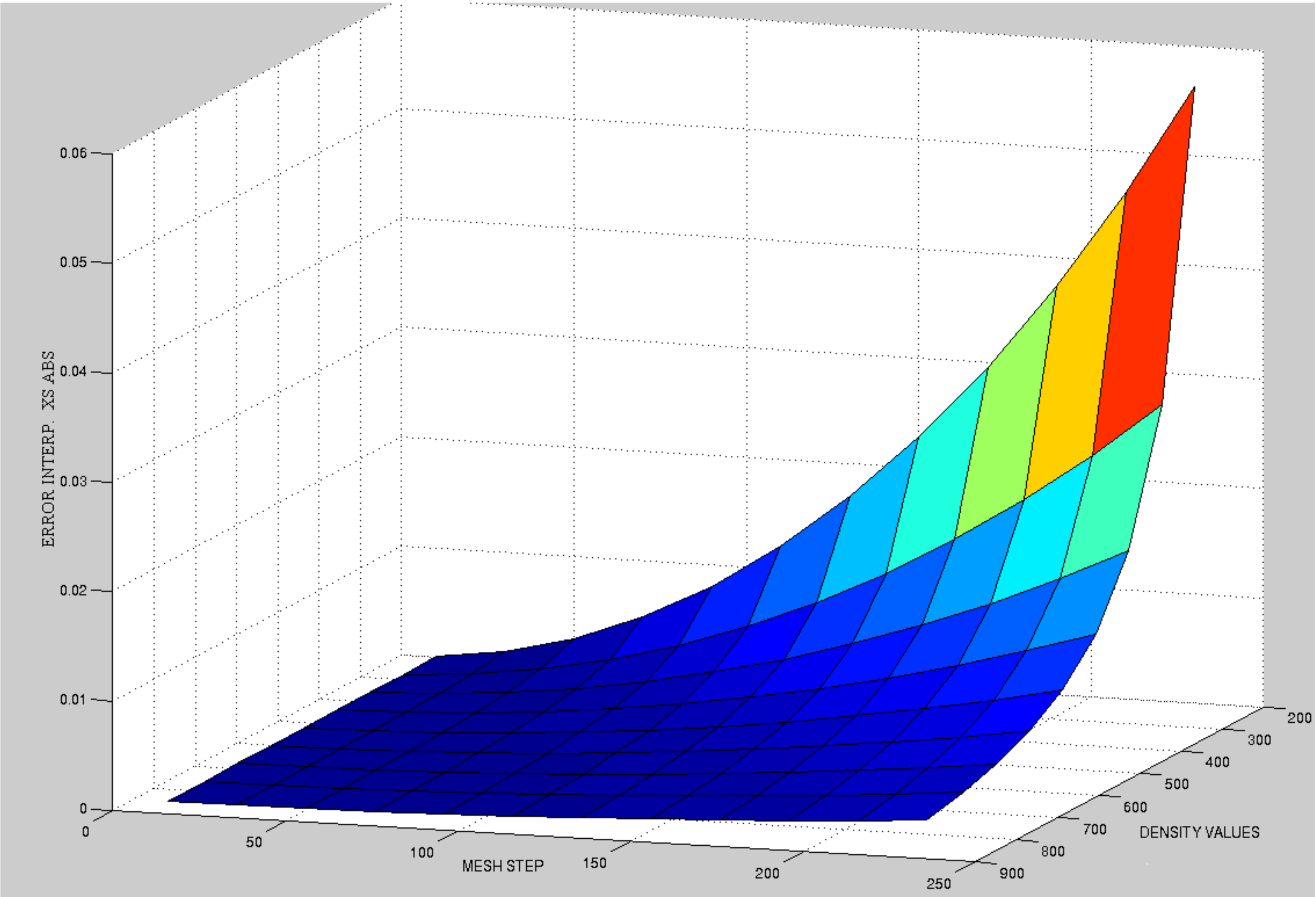
$$\vdots$$

$$\varepsilon_{\text{int}M}(\rho_M) = \Sigma(\rho_M) - \sum_{i=1}^{N+1} a_i \rho^{i-1}$$



- Interpolation error needs to be reduced if it is larger than such target error

Methodology



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Optimization process

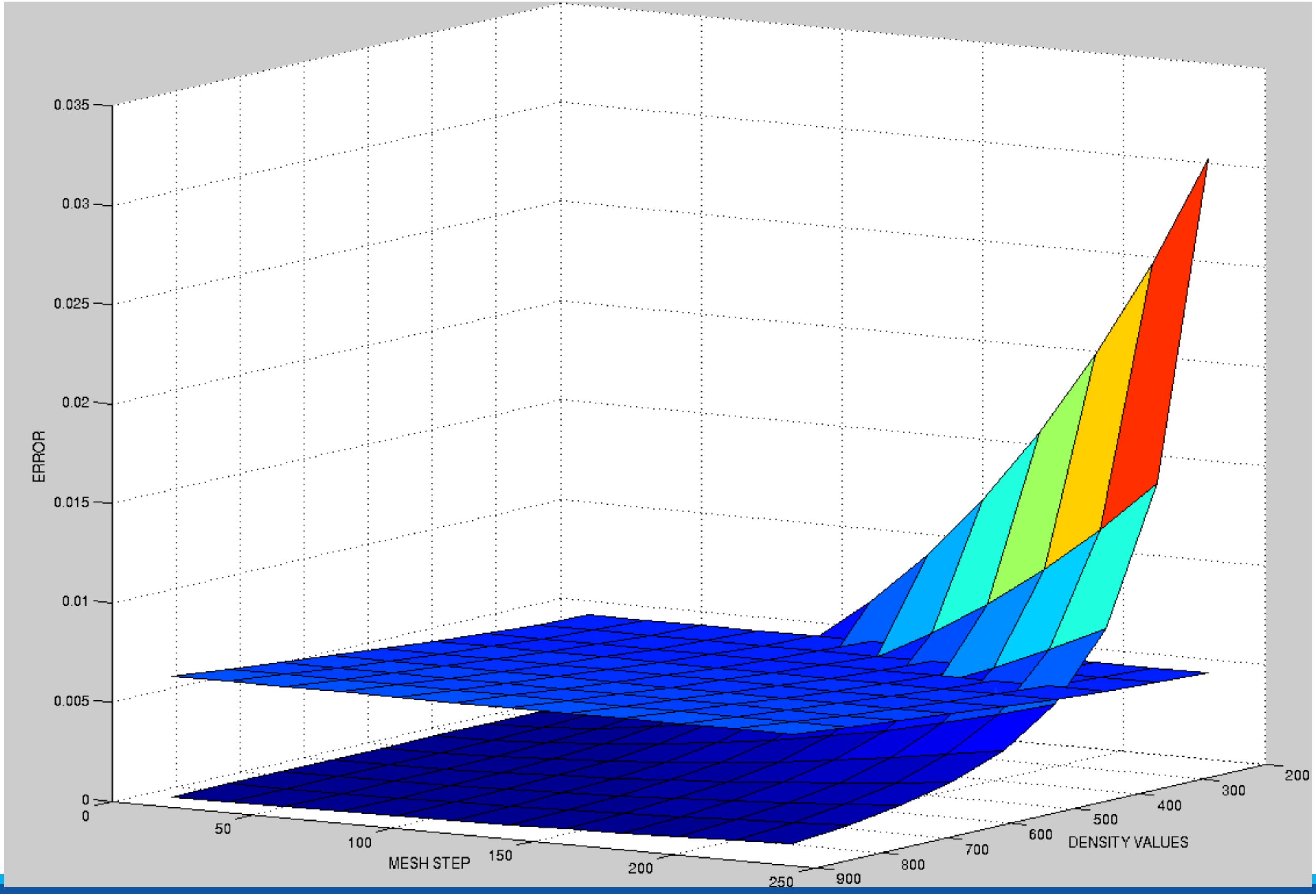
- An optimization problem is resolved: the intersection between the surface defined by the XS interpolation error with the target error defines the optimal point distribution

$$\varepsilon_{\text{int}1}\left(\rho_1\right)=\Sigma\left(\rho_1\right)-\sum_{i=1}^{N+1} a_i \rho^{i-1} \le \varepsilon_{obj}\left(\rho_1\right)$$

$$\vdots$$

$$\varepsilon_{\text{int}\,M}\left(\rho_M\right)=\Sigma\left(\rho_M\right)-\sum_{i=1}^{N+1} a_i \rho^{i-1} \le \varepsilon_{obj}\left(\rho_M\right)$$

Optimization process



Optimization process

- In fact, k-eff depends on all cross sections; the error in k-eff has to take into account all the contributions:

$$\mathbf{var}(\boldsymbol{k}) = (\Delta \boldsymbol{k})^2 = \mathbf{S}[\boldsymbol{COV}]\mathbf{S}^{\boldsymbol{T}}$$

- Where **S** refers to the sensitivity coefficient vector and **[COV]** to the covariance matrix. M is the number of different cross-sections (taking into account the number of energy groups). Correlation between XS is not considered

$$\boldsymbol{S} = \begin{bmatrix} \frac{\partial k}{\partial \Sigma_1} & \cdots & \frac{\partial k}{\partial \Sigma_j} & \cdots \end{bmatrix} \qquad [COV] = \begin{bmatrix} \delta\Sigma_1^2 & \cdots & & & \\ \vdots & \ddots & & & \\ & & \delta\Sigma_j^2 & & \\ & & & \ddots & \\ & & & & \delta\Sigma_M^2 \end{bmatrix}$$

- An automatic procedure has been set up in order to determine the optimal point distribution

Results

- The procedure has been applied to the analysis of the rod ejection transient of the *OECD/NEA and U.S. NRC PWR MOX/UO_2 core transient benchmark*
- Core loading pattern:
  - 2 types of fuel (MOX/UOX), different enrichment, different burnup, controlled/uncontrolled
  - 20 fuel assembly types

	1	2	3	4	5	6	7	8
A	U 4.2% (CR-D) 35.0	U 4.2% 0.15	U 4.2% (CR-A) 22.5	U 4.5% 0.15	U 4.5% (CR-SD) 37.5	M 4.3% 17.5	U 4.5% (CR-C) 0.15	U 4.2% 32.5
B	U 4.2% 0.15	U 4.2% 17.5	U 4.5% 32.5	M 4.0% 22.5	U 4.2% 0.15	U 4.2% (CR-SB) 32.5	M 4.0% 0.15	U 4.5% 17.5
C	U 4.2% (CR-A) 22.5	U 4.5% 32.5	U 4.2% (CR-C) 22.5	U 4.2% 0.15	U 4.2% 22.5	M 4.3% 17.5	U 4.5% (CR-B) 0.15	M 4.3% 35.0
D	U 4.5% 0.15	M 4.0% 22.5	U 4.2% 0.15	M 4.0% 37.5	U 4.2% 0.15	U 4.5% (CR-SC) 20.0	M 4.3% 0.15	U 4.5% 20.0
E	U 4.5% (CR-SD) 37.5	U 4.2% 0.15	U 4.2% 22.5	U 4.2% 0.15	U 4.2% (CR-D) 37.5	U 4.5% 0.15	U 4.2% (CR-SA) 17.5	
F	M 4.3% 17.5	U 4.2% (CR-SB) 32.5	M 4.3% 17.5	U 4.5% (CR-SC) 20.0	U 4.5% 0.15	M 4.3% 0.15	U 4.5% 32.5	
G	U 4.5% (CR-C) 0.15	M 4.0% 0.15	U 4.5% (CR-B) 0.15	M 4.3% 0.15	U 4.2% (CR-SA) 17.5	U 4.5% 32.5		
H	U 4.2% 32.5	U 4.5% 17.5	M 4.3% 35.0	U 4.5% 20.0				

Assembly Type
CR Position
Burnup [GWd/t]
Fresh
Once Burn
Twice Burn

CR-A
CR-B
CR-C
CR-D
CR-SA
CR-SB
CR-SC
CR-SD
O

Rod ejected is position E5

Results: building optimized mesh

- For each FA type, the benchmark provided a library for the following mesh:

Fuel Temp. (K)	560	900	1320
Boron conc. (ppm)	0	1000	2000
Density (kg/m³)	661.14	711.87	752.06

Benchmark mesh

- An optimized mesh has been built in 2 energy groups for the following FA types:
  - UOX-4.2w/o fresh fuel & twice burned
  - UOX-4.5w/o fresh fuel & twice burned
  - MOX-4.0w/o fresh fuel & twice burned
  - MOX-4.3w/o fresh fuel & twice burned
- It has been demonstrated that it is possible to use the same mesh for those FA types with no penalization

Fuel Temp. (K)	560	655	775	915	1035	1155	1280	1390
Boron Conc. (ppm)	1010		1390			1805		
Density (kg/m³)	661		693		726		760.5	

Optimized mesh for Δk=5pcm

Results: Part III-Steady-state at HZP previous to the transient (critical boron concentration search)

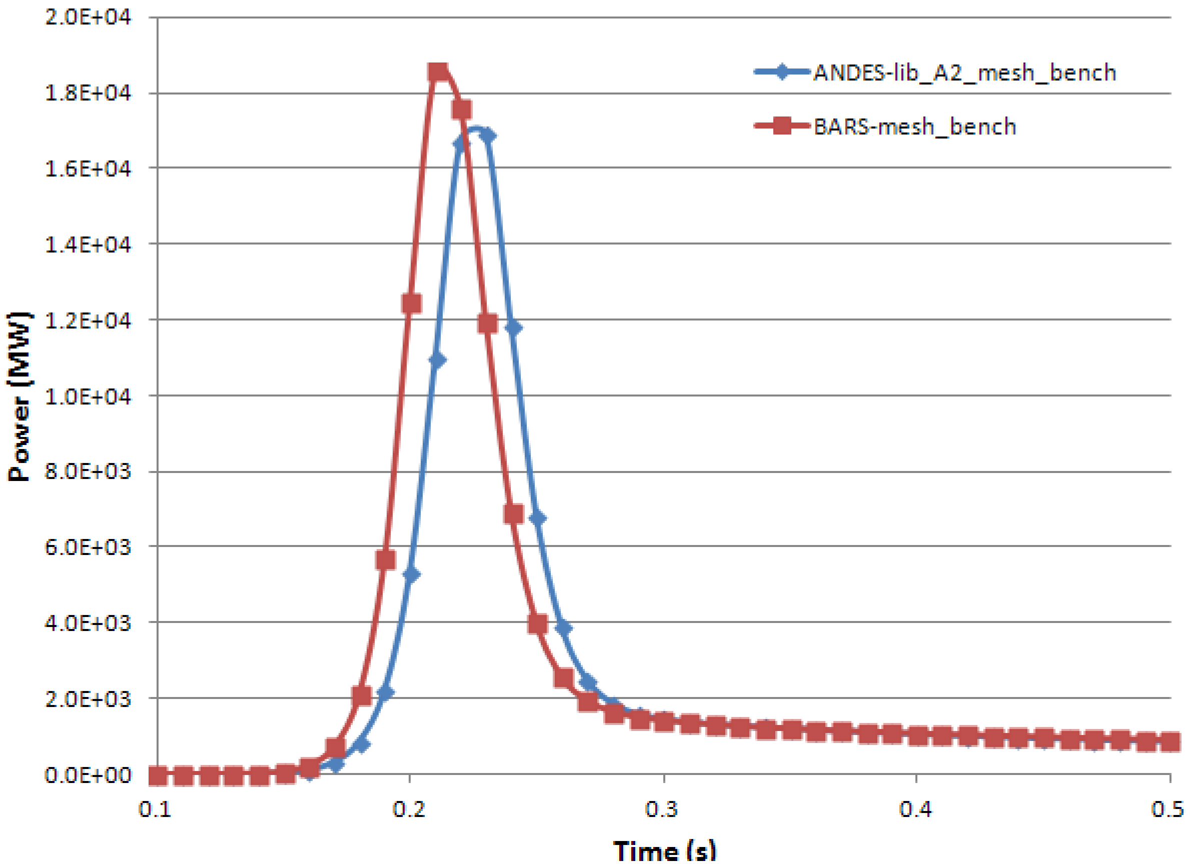
- Comparison between ANDES (COBAYA3) solution with the reference code DeCART (Heterogeneous reference solution, 47G MOC) using:
  - Mesh provided in the benchmark specifications
  - Optimized meshes

Code	Mesh	Boron concentration (ppm)
ANDES 2G	*benchmark*	1292.2
	optimized (Δk=25 pcm)	1269.9
	optimized (Δk=5 pcm)	1268.7
DeCART		1265.0

  - When de number of mesh data-points increases, the critical boron concentration converge gradually to the reference value provided by DeCART

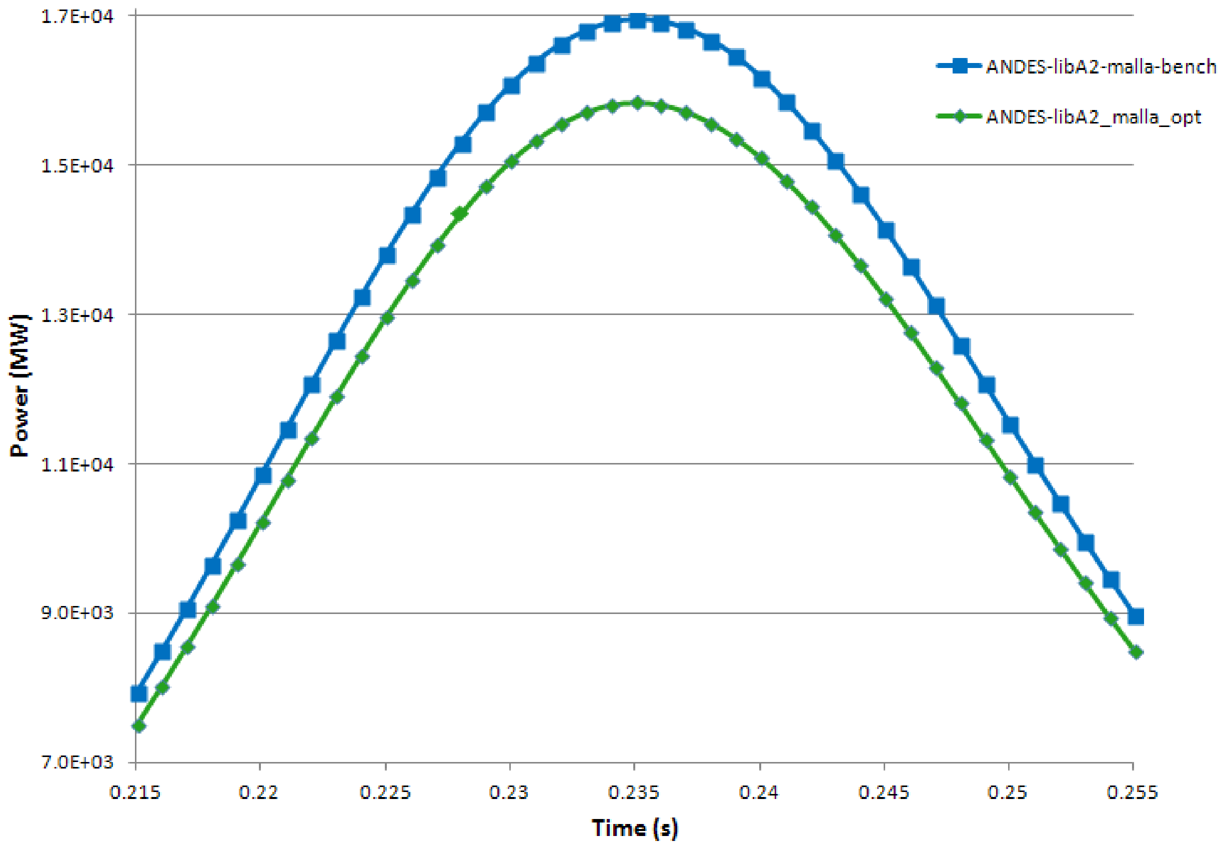
Results: Part IV-Transient rod ejection from HZP

- Transient response to control rod ejection in 0.1 s
- ANDES+COBRA-TF solution (2G, 4 N/FA, Δt = 0.005 s) is compared to other participants solutions (BARS) when using the benchmark mesh



Results: Part IV-Transient rod ejection from HZP

- ANDES+COBRA-TF solutions are compared when using two different meshes: the optimized one and the benchmark mesh
- **DIFERENCES AROUND 7%**



Conclusions

- A new process to optimize XS tabulated libraries based on the use of sensitivity coefficients has been developed

- Optimization allows increasing or reducing the distance between mesh points according to their impact over k-eff parameter

- This is a first application of the sensitivity coefficients obtained with COBAYA3 code thanks to the recent implementation of ASAP methodology

- In the context of UAM project these coefficients are going to be used for the uncertainty propagation to final results: k-eff, radial power distribution, pin-power, … (in progress)

Thanks for your attention